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13. ABSTRACT (Maximum 200 words) This project explores homogenization-based design as a systematic approach to the optimization of high-porosity materials and structures. We have shown that when the goal is maximal stiffness, extremal effective behavior does not require multiscale architecture. In fact, optimal structures can be found within a simple class of closed-cell, high-porosity composites we call “single-scale laminates.” Moreover there is a simple formula for the Hooke’s law of a single-scale laminate. It reduces the task of structural optimization for minimum weight and maximal stiffness to a convex optimization – specifically, a problem of semidefinite programming. The optimal structures are not in general unique – indeed, there is a high degree of degeneracy. It is natural to use simplicity and/or continuity as selection mechanisms. We have developed efficient schemes for doing so. <div style="text-align: right; font-size: 2em; font-weight: bold;">20040810 061</div>				
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Optimization of Structural Topology in the High-Porosity Regime

Final progress report on DAAD19-00-1-0384, July 1, 2000 – June 30, 2003

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Abstract

This project applied homogenization-based methods to the optimization of high-porosity materials and structures. We have shown that when stiffness is preferred, extremal effective behavior does not require multiscale architecture in the high-porosity limit. Rather, extremal structures can be found within the simple class of closed-cell composites we call “single-scale laminates.”

Concerning the design of optimal materials, we address the following problem: given a “target Hooke’s law” C_1 , find the minimum density of a porous composite whose effective Hooke’s law C satisfies $C \geq C_1$. We focus on the high-porosity limit, i.e. the leading-order behavior when C_1 is close to 0. Our assertion is that minimizing density over all composites is equivalent to minimizing it over single-scale laminates. Moreover finding an optimal single-scale laminate is easy – it amounts to a problem of semidefinite programming. This optimization is rather degenerate – its solution is far from unique – so it is natural to impose a selection criterion, for example maximizing manufacturability. A numerically effective selection scheme is to maximize a linear function over the class of eligible single-scale laminates. This involves solving a linear programming problem, and leads to single-scale laminates using just a few lamination directions.

For the design of optimal structures, we apply a similar strategy. However in this setting the target Hooke’s law varies in space on the macroscopic length scale. Therefore it is natural to seek optimal single-scale laminates whose layering directions vary continuously in space. This requires a different, more global selection criterion. Our solution involves solving a quadratic programming problem – minimizing, roughly speaking, the Dirichlet norm of the gradient of the single-scale laminates, subject to the constraint that they be pointwise optimal.

Subject terms: optimal design, composite materials, high-porosity structures

1 Problem statement

This project unified two themes that were previously considered quite separate: (i) the analysis of ultra-lightweight structures, and (ii) homogenization-based optimal design.

The first theme has attracted a lot of attention in the materials community [6, 8, 10]. Work has mainly focused on analyzing specific classes of light-weight structures, of biological, physical, or synthetic origin – such as bone, wood, periodic lattices, and random foams.

The second theme has attracted a lot of attention in the mathematics community [1, 4, 5]. Work has mainly focused on minimizing weight and maximizing stiffness. Remarkably, the mathematical theory does much more than merely optimize the sizing of structural members; it also identifies the optimal structural topology.

Our insight was that the homogenization-based theory should simplify in the high-porosity limit, where the goal is to design ultra-lightweight structures. This has proved to be the case. In general, the optimal microstructures provided by the homogenization-based theory are complicated, and in some regimes they require multiple length scales. In the high-porosity limit, however, we have found that relatively simple structures are optimal to leading order.

Our accomplishments go far beyond specializing the homogenization-based theory to the high-porosity regime. The optimal structures are “single-scale laminates,” whose Hooke’s laws depend linearly on the laminate thicknesses. Numerical structural optimization in this regime is much easier than the general case, because it reduces to convex optimization.

The simplest version of the design problem minimizes density over the class of porous composites whose effective Hooke’s law C satisfies $C \geq C_1$, for a given “target Hooke’s law” C_1 . To focus on the high-porosity limit, we study the leading-order behavior when C_1 is close to 0. When we say that “the optimal structures are single-scale laminates” we mean that minimizing density over all porous composites is equivalent to minimizing it over single-scale laminates. Numerically, this reduces to a problem of semidefinite programming.

The optimization over single-scale laminates is rather degenerate: there are, in fact, many optimal structures. It is therefore natural to impose a selection criterion that favors manufacturability. A numerically effective selection scheme is to maximize a linear function over the class of eligible single-scale laminates. This involves solving a linear programming problem, and leads to single-scale laminates that use just a few lamination directions.

A similar strategy can be applied to the design of (heterogeneous) structures. In that setting, however, the target Hooke’s law varies in space on the macroscopic length scale. Therefore it is natural to seek optimal structures which are locally single-scale laminates, with continuously varying layer directions and densities. This is a more global selection criterion. Our approach to solving it minimizes, roughly speaking, the Dirichlet norm of the gradient of the single-scale laminates, subject to the constraint that they be pointwise optimal. This reduces numerically to a large quadratic programming problem.

2 Summary of main results

2.1 Definition of a single-scale laminate

We focus exclusively on high-porosity composites made from a fixed elastic material with Hooke's law A .

The simplest example of such a composite is a *layered structure* with layering direction k and density θ . Its microstructure consists of layers of material A , separated by void. The layers are perpendicular to the unit vector k , with thicknesses and spacing chosen so the overall volume fraction of material is $\theta > 0$. (The high-porosity limit corresponds to $\theta \rightarrow 0$.) The effective Hooke's law of the resulting composite is clearly degenerate, since stress is only produced by the components of the strain "tangent to the layers." Its formula is well-known [1, 9]. The Hooke's law is proportional to θ , so it has the form $\theta f(k)$, where the function f is defined on unit vectors, taking values in the space of Hooke's laws. When A is isotropic, i.e. $A\xi = 2\mu_A\xi + \lambda_A(\text{tr}\xi)I$, we have

$$\langle f(k)\xi, \xi \rangle = \langle A\xi, \xi \rangle - \frac{1}{\mu_A}|A\xi k|^2 + \frac{\lambda_A + \mu_A}{\mu_A(\lambda_A + 2\mu_A)}\langle A\xi k, k \rangle^2.$$

For a general, possibly anisotropic A , the corresponding formula is

$$f(k)\xi = A^{1/2}\Pi_{A^{-1/2}W(k)}A^{1/2}\xi, \quad (1)$$

where Π_X denotes orthogonal projection onto the subspace X , and $W(k)$ is the space of stresses compatible with layering direction k :

$$W(k) = \{\eta : \eta \cdot k = 0\}.$$

The structures considered above have just one family of layers, i.e. a single layering direction. Our *single-scale laminates* are similar, but they have layers in many directions rather than just one. A single-scale laminate is characterized by its

$$\text{layering directions } k_1, \dots, k_p,$$

which must be unit vectors, and its

$$\text{relative densities } t_1, \dots, t_p,$$

which must be positive with $t_1 + \dots + t_p = 1$. The microstructure consists of p families of walls, the i th family being orthogonal to k_i with density $t_i\theta$. In the high-porosity limit, when $\theta \rightarrow 0$, the volume where the walls overlap is negligible, so the density of the entire structure is, to leading order, $\theta t_1 + \dots + \theta t_p = \theta$.

Some special cases are very familiar. In two space dimensions, a square lattice is a single-scale laminate with $k_1 = (1, 0)$, $k_2 = (0, 1)$ and $t_1 = t_2 = 1/2$. Similarly, a triangular lattice is realizable as a single-scale laminate with $t_1 = t_2 = t_3 = 1/3$. We have specified the layering directions but not their positions relative to one another; the Kagome lattice [11] has the same layering directions and densities as the triangular lattice, but only two members meet at each vertex; it too is a single-scale laminate. Our results show that the

Hooke's law depends only on the layering directions and densities in the high-porosity limit; other microstructural details, like those that distinguish the Kagome and triangular lattices, are irrelevant at leading order.

Notice that in three space dimensions a single-scale laminate consists of walls. It cannot have one-dimensional members. Thus a closed-cell cubic structure with walls orthogonal to each coordinate axis is an example of a single-scale laminate; however a truss-like structure with struts along the coordinate axes and diagonals is *not* a single-scale laminate. Our results show that when maximal stiffness and minimum weight are preferred, it is not a good idea to consider truss-like structures in 3D. The intuitive reason is this: a wall is multifunctional – it resists stresses in every in-plane direction – whereas a one-dimensional member can only resist stress in its tangent direction.

2.2 The Hooke's law of a single-scale laminate

The effective Hooke's law of a single-scale laminate has an extremely simple formula: it is simply

$$C = \theta \sum_{i=1}^p t_i f(k_i). \quad (2)$$

This is a bit surprising. Each family of walls can be viewed as a substructure, with scaled Hooke's law $t_i f(k_i)$. Equation (2) says their Hooke's laws are additive. This would be clear if the walls were independent, like springs in parallel. But they are not entirely independent, because walls in different directions intersect. These intersections would appear to impose additional constraints, since the elastic displacement must be continuous. The assertion of (2) is that these constraints are negligible at leading order in the high-porosity limit.

We briefly sketch the proof of (2). One inequality is easy: if the effective Hooke's law is C then

$$C \geq \theta \sum_{i=1}^p t_i f(k_i)$$

since the right hand side is what we get by ignoring the constraint of kinematic compatibility at the intersections of the walls. The opposite inequality is proved using the Hashin-Shtrikman variational principle, which gives an upper bound for C in terms of the H -measure associated with its microstructure. In the high-porosity limit this H -measure is easy to compute and the bound reduces to $C \leq \theta \sum_{i=1}^p t_i f(k_i)$.

2.3 Optimality of single-scale laminates

We claim that when the goal is optimal design for minimum weight in the high-porosity regime, if in addition stiffness is preferred, then there is no need to look beyond the class of single-scale laminates.

Here is a mathematically precise statement of this result. Consider any porous composites made from material A and void, with overall volume fraction θ of material, and let C_1 be its effective Hooke's law. We claim there exists a single-scale laminate with the *same* volume fraction θ (to leading order) whose Hooke's law C satisfies

$$C \geq C_1.$$

Thus if stiffness is preferred (i.e. if C is at least as good as C_1 for the given design purpose) the search for minimum-weight structures in the high-porosity limit can safely be restricted to single-scale laminates.

The proof of this result is parallel to Avellaneda's demonstration that optimal structures can be found, at any density, within the class of sequential laminates [2]. The main novelty is the observation that in the high-porosity limit there is no need for separation of scales. Indeed, for any sequential laminate we can consider the single-scale laminate with the same layering directions and densities; their Hooke's laws turn out to be identical at leading order as $\theta \rightarrow 0$.

Besides demonstrating optimality, the equivalence of sequential laminates and single-scale laminates in the high-porosity limit has a useful byproduct. It leads to an algorithm for calculating, for any given macroscopic stress or strain, the local stress and strain in each wall of a single-scale laminate.

2.4 Numerical optimization over single-scale laminates

We have shown that for certain optimal design problems, there is no need to look beyond the class of single-scale laminates. Now let's take advantage of this observation.

Let C_1 be a given "target" Hooke's law, and consider the minimum-weight design of a single-scale laminate subject to the constraint that its Hooke's law is stiffer than C_1 . Mathematically: this amounts to the optimization

$$\min \left\{ \sum_{i=1}^p \tau_i : \tau_i \geq 0; |k_i| = 1; \sum_{i=1}^p \tau_i f(k_i) \geq C_1 \right\}. \quad (3)$$

Here τ_i plays the role of θt_i , so $\sum_i \tau_i = \theta$ is the density of the composite. Both the objective and the constraints are homogenous of degree one, so it is not actually necessary that C_1 be near 0. Rather, C_1 represents the leading order behavior of the desired single-scale laminate, and $\tau_j / \sum_{i=1}^p \tau_i$ represents the relative density of the j th wall. We do not know in advance which layering directions will be useful, so the vectors $\{k_i\}_{i=1}^p$ should be evenly distributed on the unit sphere (for 3D calculations) or the unit circle (in 2D). All our numerical experiments were done in 2D.

The unknowns in (3) are $\{\tau_i\}_{i=1}^p$. (We hold the vectors k_i fixed). At first (3) looks like a linear programming problem, since the objective is linear and each τ_i is nonnegative. But actually it is a *semidefinite programming problem*, since the constraint $\sum_{i=1}^p \tau_i f(k_i) \geq C_1$ asks that a certain matrix (depending linearly on the τ_i) be positive semidefinite. No problem: this class of convex optimization problems is now well understood. We solved (3) using a standard software package based on an interior point method.

2.5 Selecting a single-scale laminate with few layering directions

In practice, the solution of (3) found using the interior point method has $\tau_i > 0$ for every i . This is not surprising – it is in fact what we *expect* of an interior point scheme.

The numerical solution is robust, and it reflects the symmetries of C_1 ; for example, if C_1 is isotropic and the directions k_i are evenly spaced then the optimal τ_i are independent of i .

Practically speaking, however, the manufacturability of a single-scale laminate should be related to the number of distinct layering directions. Therefore it is natural to seek a different solution in which most of the τ_i are 0. An effective means for achieving this is to maximize the density of the layers in a particular direction. We do this by solving

$$\max \left\{ \tau_1 : \tau_i \geq 0; \sum_{i=1}^p \tau_i = \theta; \sum_{i=1}^p \tau_i f(k_i) = C \right\} \quad (4)$$

where C is the Hooke's law of the single-scale-laminate obtained by solving (3) and θ is its density.

The optimization (4) is a standard linear programming problem. Indeed, its unknowns τ_i are nonnegative. The constraint $\sum_{i=1}^p \tau_i f(k_i) = C$ is now understood pointwise, so it is simply a collection of linear equality constraints. The constraint is feasible, by the choice of C , and the objective is linear.

The solution of (4) is observed numerically to have just a few nonzero τ_i 's. This is no surprise: the optimal value of a linear program is achieved, barring degeneracy, at an extreme point of the feasible set. Therefore solving (4) should drive as many τ_i as possible to zero; the number that remain nonzero is determined by the number of equality constraints.

The ordering of the layering directions is of course arbitrary. As we vary the direction of k_1 , (4) produces a large family of *different* single-scale laminates with few layering directions and the same Hooke's law C .

2.6 Continuous spatial variation

We have focused thus far on problems of *material design*: for a given target Hooke's law, we have sought minimum-weight structures that achieve (or exceed) the target rigidity to leading order in the high-porosity limit. The target Hooke's law was constant, and the optimal single-scale laminates were spatially periodic.

What about problems of *structural design*, where the loads and boundary conditions are not uniform on the macroscopic length scale? The homogenization-based approach to structural optimization addresses such problems in two steps:

- (1) identify the spatially-varying macroscopic Hooke's law of an optimal structure, then
- (2) construct an associated microstructure, by using composites whose microstructural characteristics vary on the macroscopic length scale.

The steps are of course coupled, since the first requires that we know the "cost" of achieving a given Hooke's law. An appealing implementation of step (1) was given in [3] using semidefinite programming. But that work used a simple phenomenological formula for the "cost" of a Hooke's law, and made no attempt to address step (2).

Our results complement those of [3] by providing a rational cost function. For example, suppose the goal is to minimize weight with constraints on the compliance of the structure under a variety of specified loads. Then rigidity is preferred, and our Eqn (3) gives the cost associated with any Hooke's law C_1 in the high-porosity limit. The resulting implementation of step (1) would use a fixed discretization of the unit sphere $\{k_i\}_{i=1}^p$. The parameters τ_i would now be functions of x , defined at all points of the macroscopic domain

Ω occupied by the structure (more precisely: at grid or nodal points of a finite-difference or finite-element discretization of this domain). The local Hooke's law of the structure is then $C(x) = \sum_{i=1}^p \tau_i(x) f(k_i)$, and the numerical problem is to minimize $\int_{\Omega} \sum_i \tau_i$ subject to (a) the pointwise scalar constraints $\tau_i(x) \geq 0$, and (b) constraints on the structure's compliance under each specified load.

We did not actually implement the optimization just described. Rather, we have focused on what to do afterward, i.e. how to accomplish step (2). The output of step (1) would be the spatially-varying thickness parameters $\tau_i(x)$ of a single-scale laminate. We would like to specify, from such data, a design for entire structure that is (a) consistent with the optimal macroscopic density $\theta(x) = \sum \tau_i(x)$ and Hooke's law $C(x) = \sum \tau_i(x) f(k_i)$, and (b) relatively simple.

The simplification scheme discussed above in Eqn (4) can of course be applied pointwise. As x varies, this amounts to solving a family of linear programs with the same objective but varying constraints. The result is a family of single-scale laminates whose layer directions are *piecewise constant* in x . This behavior is easy to understand. Indeed, each extreme point of the admissible set for (4) corresponds to a selection of nonzero τ_i 's. As x varies, the optimum stays for a while at one extreme point, then eventually jumps to another one. The layering directions are constant in the region associated with a given extreme point; at the boundary of this region one of the layering directions disappears (its τ_i goes to 0) and another one emerges in its place.

Perhaps the structures obtained this way could be manufactured and used. However our instinct is that discontinuities should be avoided whenever possible. Therefore we sought an alternative selection scheme which would make the layering directions and their thicknesses vary continuously with x . For simplicity we took Ω to be an interval $[0, 1]$, and we chose $C(x)$ by taking $C_1(x)$ to interpolate linearly between two Hooke's laws A_0 and A_1 , then solving (3) at each spatial grid point.

To promote continuity one must discuss all values of x simultaneously. So the unknown is really a parametrized measure τ_x , defined for $x \in \Omega$ and taking values in the space of positive measures on the unit sphere S , such that $\int_S d\tau_x(k) = \theta(x)$ and $\int_S f(k) d\tau_x(k) = C(x)$ for all x . We want designs with few distinct layering directions, so it is natural to restrict τ_x to consist of a small number (say, M) of point masses. The selection scheme should favor continuous dependence, so it is natural to optimize a sort of Dirichlet norm

$$\min \sum_{j=1}^{N-1} \text{dist}^2(\tau_{x_j}, \tau_{x_{j+1}}). \quad (5)$$

Here $\{x_j\}_{j=1}^N$ are grid points in Ω ; each τ_{x_j} is a positive measure with at most M point masses; and we must respect pointwise linear constraints to assure that τ_{x_j} has the right mass and Hooke's law at each grid point.

To specify the scheme completely, we must say (a) how to discretize the τ_{x_j} 's, and (b) how to evaluate $\text{dist}(\tau_{x_j}, \tau_{x_{j+1}})$. The answer to (a) is simple: we represent each measure τ_{x_j} by an unordered collection of pairs $(k_1, m_1), \dots, (k_M, m_M)$ where each k_i is a unit vector and $m_i \geq 0$. (The measure has mass m_i at unit vector k_i .) As for (b): we found it convenient to take

$$\text{dist}(\tau, \tau') = \|f * (\tau - \tau')\|_{L^2(S)}$$

where f is positive, unimodal function with L^1 norm one. With these interpretations the optimization (5) becomes a large quadratic programming problem. It can be solved quite easily using a standard QP code. Our numerical experiments show that the resulting designs have the desired characteristics: they are locally single-scale laminates, which achieve the desired density and Hooke's law using just a few layering directions which vary continuously with x .

2.7 Discussion

Our goal was to exploit homogenization-based methods for the optimal design of high-porosity structures. We have in large measure achieved this goal, for problems in which stiffness is preferred and the objective is weight minimization.

There are, of course, optimal design problems where stiffness is not preferred. The design of a composite for minimum Poisson's ratio is an example. Assuming isotropy, this objective requires a large shear modulus but a small bulk modulus. It is known that a porous composite can have any Poisson's ratio consistent with positivity of the Hooke's law [7]. However the Hooke's law of an isotropic single-scale laminate is entirely determined by its density, and its shear and bulk modulus achieve the (high-porosity limit of the) Hashin-Shtrikman bounds. Thus our method cannot be used to optimize the weight of a negative-Poisson-ratio material. If we solve (3) with a target Hooke's law C_1 for which Poisson's ratio is negative, the resulting single-scale laminate will have a positive Poisson ratio. This difficulty is not special to the high-porosity regime: it is a well-known limitation of the homogenization-based method [1].

The subject remains at a very preliminary stage of development. We have suggested combining our results with the method of [3] but this proposal remains to be implemented. We have shown how to select simple single-scale laminates with continuous spatial dependence, but we have not examined the properties of the resulting structures – for example their resistance to buckling. Thus, like any good research project, our investigation has raised as many questions as it answered.

3 Publications and presentations

Papers published in refereed journals: We intend to write at least two articles based on this work. One, targeted toward the applied mathematics community working in homogenization and structural optimization, will emphasize the theory. The other, targeted toward the large mechanics community doing structural optimization, will emphasize the conclusions and numerical examples.

Conference proceedings:

1. Blaise A. Bourdin and Robert V. Kohn, *Extremal light-weight microstructures*, Proc. 15th ASCE Engineering Mechanics Conference, June 2-5, 2002, Columbia University, New York

Conference presentations without proceedings:

1. Blaise A. Bourdin and Robert V. Kohn, *Elastically optimal microstructures in the high-porosity regime*, Fourteenth U.S. National Congress on Theoretical and Applied Mechanics, Blacksburg, VA, June 23-28 2002. Invited talk in Symposium on Advances on Composite Materials.
2. Blaise Bourdin and Robert V. Kohn, *Extremal high-porosity microstructures*, First Joint Meeting of the AMS and UMI, Pisa, Italy, June 12-16, 2002. Invited talk in Special Session "Some Mathematics around Composites."
3. Blaise Bourdin and Robert V. Kohn, *Elastically optimal microstructures in the high-porosity regime*, Fourth SIAM Conference on Mathematical Aspects of Materials Science, May 23-26, 2004. Invited talk in the Minisymposium "Composites and Polycrystals."

4 Scientific personnel

The project budget was devoted almost exclusively to salary for a postdoctoral researcher, Blaise Bourdin. Blaise is now a tenure-track Assistant Professor of Mathematics at Louisiana State University.

5 Report of inventions

This project did not lead to new patents or inventions.

6 Service

The PI chaired the Board of Visitors at the May, 2001 Program Review of ARO's Basic Research Program in Mathematics.

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